Acenaphthylene, 5-bromo-1,2-dihydro-

Other names:	5-Bromoacenaphthene
	Acenaphthene, 5-bromo-
Inchi:	InChI=1S/C12H9Br/c13-11-7-6-9-5-4-8-2-1-3-10(11)12(8)9/h1-3,6-7H,4-5H2
InchiKey:	QALKJGMGKYKMKE-UHFFFAOYSA-N
Formula:	C12H9Br
SMILES:	Brc1ccc2c3c(cccc13)CC2
Mol. weight [g/mol]:	233.10
CAS:	2051-98-1

Physical Properties

Property code	Value	Unit	Source
gf	335.21	kJ/mol	Joback Method
hf	227.81	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.701		Crippen Method
mcvol	143.360	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	608.20	K	NIST Webbook
tb	608.50 ± 0.50	K	NIST Webbook
tc	864.13	K	Joback Method
tf	407.18	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.44	J/mol×K	864.13	Joback Method
cpg	326.51	J/mol×K	650.57	Joback Method
cpg	337.59	J/mol×K	693.28	Joback Method
cpg	347.76	J/mol×K	735.99	Joback Method
cpg	357.18	J/mol×K	778.70	Joback Method
cpg	366.02	J/mol×K	821.41	Joback Method

cpg	314.34	J/mol×K	607.86	Joback Method
dvisc	0.0018241	Pa×s	407.18	Joback Method
dvisc	0.0015639	Pa×s	440.63	Joback Method
dvisc	0.0013702	Pa×s	474.07	Joback Method
dvisc	0.0012216	Pa×s	507.52	Joback Method
dvisc	0.0011047	Pa×s	540.97	Joback Method
dvisc	0.0010108	Pa×s	574.41	Joback Method
dvisc	0.0009339	Pa×s	607.86	Joback Method
hsubt	87.40 ± 2.60	kJ/mol	308.00	NIST Webbook
psub	2.77e-04	kPa	311.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	5.63e-05	kPa	298.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.07e-04	kPa	303.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	1.44e-04	kPa	305.70	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

psub	1.84e-04	kPa	308.00	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	3.92e-05	kPa	295.50	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	3.44e-04	kPa	314.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	4.35e-04	kPa	316.60	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	
psub	5.60e-04	kPa	318.90	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique	

psub	5.53e-04	kPa	319.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	7.25e-04	kPa	321.20	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique
psub	6.79e-04	kPa	321.40	The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	460.50 ± 2.50	K	2.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051981&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

The effect of halogen hetero-atoms on the vapor pressures and thermodynamics of polycyclic aromatic compounds measured via the Knudsen effusion technique: https://www.doi.org/10.1016/j.jct.2007.09.006

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume